

6-Benzyl-6,7-dihydro-5H-pyrrolo[3,4-B]pyridine
109966-30-5 | DTXSID50364043

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 312 °C

Global applicability domain: Inside

Local applicability domain index: 4.19e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Methyl-5-nitro-1H-isoindole-
1,3(2H)-dione

Measured: 361

Predicted: 323

[Image not found](#)

Acibenzolar-S-methyl

Measured: 267

Predicted: 295

[Image not found](#)

1H-Pyrazole, 3,5-dimethyl-1-
phenyl-

Measured: 273

Predicted: 287